Safety Data Sheet

Thionyl chloride

Division of Safety
National Institutes
of Health

WARNING!

THIS COMPOUND IS ACUTELY TOXIC. IT IS RAPIDLY HYDROLYZED TO HYDROCHLORIC ACID AND SULFUR DIOXIDE, AND ITS TOXIC ACTION IS THAT OF THESE SUBSTANCES. IT MAY CAUSE SEVERE IRRITATION OF TISSUES (SKIN, EYES, MUCOUS MEMBRANES, AND LUNGS) AND INDUCE SENSITIVITY. AVOID FORMATION AND BREATHING OF AEROSOLS OR VAPORS.

LABORATORY OPERATIONS SHOULD BE CONDUCTED IN A FUME HOOD, GLOVE BOX, OR VENTILATED CABINET.

AVOID SKIN CONTACT: IF EXPOSED, WASH WITH SOAP AND COLD WATER. AVOID RUBBING OF SKIN OR INCREASING ITS TEMPERATURE.

FOR EYE EXPOSURE, IRRIGATE IMMEDIATELY WITH LARGE AMOUNTS OF WATER OR SODIUM BICARBONATE SOLUTION. FOR INGESTION, DRINK MILK OR WATER. REFER FOR GASTRIC LAVAGE. FOR INHALATION, REMOVE VICTIM PROMPTLY TO CLEAN AIR. ADMINISTER RESCUE BREATHING IF NECESSARY. REFER TO PHYSICIAN.

IN CASE OF LABORATORY SPILL, WEAR PROTECTIVE CLOTHING DURING CLEANUP. AVOID SKIN CONTACT OR BREATHING OF AEROSOLS OR VAPORS. USE WATER TO DISSOLVE COMPOUND. USE ABSORBENT PAPER TO MOP UP SPILL. WASH DOWN AREA WITH SOAP AND WATER. DISPOSE OF WASTE SOLUTIONS AND MATERIALS APPROPRIATELY.

A. Background

Thionyl chloride is a colorless to pale yellow fuming liquid with a suffocating odor, highly corrosive to metals. It is miscible with many organic solvents. In the presence of water it is quickly hydrolyzed to hydrochloric acid and sulfur dioxide, and its toxic effects (strong irritating and corrosive effects on skin, eyes, and mucous membranes) are due to formation of these hydrolysis products.

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Prepared by the Environmental Control and Research Program

This data sheet is provided by the Division of Safety, NIH, to accompany the *NIH Guidelines for the Laboratory Use of Chemical Carcinogens*. The information included in this document is believed to be current and accurate, but no warranty is expressed or implied.

It is used in organic synthesis (conversion of acids to acid chlorides in the manufacture of herbicides, drugs, and vitamins), in lithium batteries for pacemakers, and as a drying agent in the manufacture of optical fibers.

The permissible exposure limit to thionyl chloride is 5 mg/m^3 as a time-weighted, 8-hour average (ACGIH, 1987).

Chemical and Physical Data

1. Chemical Abstracts No.: 7719-09-7.

2. Synonym: Sulfurous oxychloride.

3. Chemical structure and molecular weight: $SOCl_2$; 118.98.

4. Density: $d_4^{20} = 1.638$.

5. Absorption spectroscopy: No characteristic peaks in the ultraviolet region (Koch, 1949); the infrared spectrum has been published (Martz and Lagemann, 1954).

6. Volatility: Vapor pressure data over the range of 1 mm - 760 mm Hg are listed on p. D-202 in Weast (1982).

7. Solubility: Thionyl chloride is miscible with many organic solvents including chlorinated and aromatic hydrocarbons (e.g., benzene, chloroform, carbon tetrachloride).

8. Description: The commercial product (99% pure) is usually pale yellow; the purified material is a colorless liquid with choking odor, fuming when exposed to the atmosphere.

9. Boiling point: 76°C; melting point: -104.5°C.

10. Stability: Storage at room temperature results in the slow formation of SO_2; it decomposes fairly rapidly above 150°C, and completely at 500°C to chlorine, sulfur dioxide, and sulfur monochloride. Reacts rapidly with water, and sometimes explosively with dimethyl sulfoxide.

11. Chemical reactivity: Thionyl chloride reacts with aliphatic compounds containing hydroxyl groups to form alkyl chlorides, sulfites, and chlorosulfites, with primary amines to form thionylamines, and with carboxylic acids to form acid chlorides or anhydrides. Its reaction with metal oxides has been used in the preparation of anhydrous metal chlorides. It is incompatible with ammonia, quinoline, and linseed oil (Sax, 1984). It attacks rubber and should therefore be manipulated (particularly when used in chemical synthesis) in all-glass apparatus. The uses of thionyl chloride in organic preparations have been reviewed (Fieser and Fieser, 1967).

12. Flash point: Thionyl chloride is nonflammable.

13. Autoignition temperature: No data.

14. Explosive limits in air: No data.

Fire, Explosion, and Reactivity Hazard Data

1. Fire fighting personnel should wear protective clothing and air-supplied respirators with full face masks.

2. Thionyl chloride is incompatible with ammonia and water.

3. Conditions contributing to instability are high temperatures.

4. Hazardous decomposition products are chlorine, hydrochloric acid, sulfur dioxide, and sulfur monochloride.

5. Since thionyl chloride is nonflammable, nonspark equipment is not required.

Operational Procedures

The NIH Guidelines for the Laboratory Use of Chemical Carcinogens describe operational practices to be followed when potentially carcinogenic chemicals are used in NIH laboratories. The NIH Guidelines should be consulted to identify the proper use conditions required and specific controls to be implemented during normal and complex operations or manipulations involving thionyl chloride.

It should be emphasized that this data sheet and the NIH Guidelines are intended as starting points for the implementation of good laboratory practices when using this compound. The practices and procedures described in the following sections pertain to the National Institutes of Health and may not be universally applicable to other institutions. Administrators and/or researchers at other institutions should modify the following items as needed to reflect their individual management system and current occupational and environmental regulations.

1. Chemical inactivation: Hydrolyzed by water or alkali.

2. Decontamination: Turn off equipment that could be affected by thionyl chloride or the materials used for cleanup. If there is any uncertainty regarding the procedures to be followed for decontamination, call the NIH Fire Department (dial 116) for assistance. Use absorbent paper to mop up spill. Wipe off surfaces with 1% sodium hydroxide or sodium carbonate, then wash with copious quantities of water. Glassware should be rinsed in a hood with sodium hydroxide solution, followed by soap and water. Animal cages should be washed with water.

3. Disposal: Waste solutions should be treated with soda ash and/or slaked lime, diluted with water, and after standing for a few hours may be disposed of in the sewer system.

4. Storage: Store thionyl chloride and its solutions in dark-colored, tightly closed, all glass containers, under refrigeration or in a freezer. Avoid exposure to light and moisture. Store working quantities of thionyl chloride and its solutions in an explosion-safe refrigerator in the work area.

Monitoring and Measurement Procedures Including Direct Field Measurements and Sampling for Subsequent Laboratory Analysis

There are no published procedures for either sampling or analysis of intact thionyl chloride, except for one seen only in abstract form (Sojecki, 1961) which consists of hydrolysis and colorimetric determination of resulting sulfur dioxide with silver nitrate. The sensitivity of this method is stated to be 0.005 mg/5 ml sample obtained from 10 liters of air. It stands to reason that other methods could be devised based on hydrolysis and estimates of chloride and/or sulfur dioxide by standard procedures.

Biological Effects (Animal and Man)

1. Absorption: Thionyl chloride is absorbed by inhalation and is a severe irritant of skin, eyes, and mucous membranes, especially those of the respiratory and alimentary tracts. There is no indication if systemic effects are produced via these routes.

2. Distribution: No data, and these are unlikely to be developed for reasons stated below.

3. Metabolism and excretion: No data. Since thionyl chloride is readily hydrolyzed *in vitro* and therefore presumably in the animal body to HCl and SO_2, its metabolic fate is that of its hydrolysis products.

4. Toxic Effects: There are no acute LD50 measurements, because of the instability of thionyl chloride in an aqueous environment. Exposure of cats for 20 minutes to 17.5 ppm thionyl chloride by inhalation was not fatal (Sax, 1984). In any event, such data would be of no practical significance since the highly suffocating odor of thionyl chloride precludes the inhalation or ingestion of a lethal dose. Symptoms of exposure are: in the eye, conjunctivitis and corneal burns possibly leading to corneal opacity; on the skin: acid burns and necrosis; in the respiratory tract: death due to asphyxia, with bronchitis and bronchopneumonia in animals surviving acute exposures. Chronic exposures to low doses produces nasopharyngitis, fatigue, and chronic symptoms of bronchitis. (These are the symptoms produced by both hydrolysis products.) In the only reported human case of accidental exposure to thionyl chloride (splashes on face and clothes) there were severe first and second degree burns of the face and spastic bronchitis which disappeared in a few days (Parmeggiani and Tagliabue, 1951).

5. Carcinogenic effects: None reported.

6. Mutagenic and teratogenic effects: None reported.

Emergency Treatment

1. Skin and eye exposure: For skin exposure, remove contaminated clothing and wash skin with soap and water. Avoid rubbing of skin or increasing its temperature. For eye exposure, irrigate immediately with dilute sodium bicarbonate solution followed by copious quantities of running water for at least 15 minutes. Obtain ophthalmological evaluation.

2. Ingestion: Drink plenty of water or milk. Refer for gastric lavage.

3. Inhalation: Remove victim promptly to clean air. Administer rescue breathing if necessary.

4. Refer to physician at once. Consider treatment for pulmonary irritation.

References

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